Computational Materials Research: Boron Suboxide Ceramic Armor

S&T Campaign: Materials Research
Tier 2 High Strain Rate & Ballistic Materials

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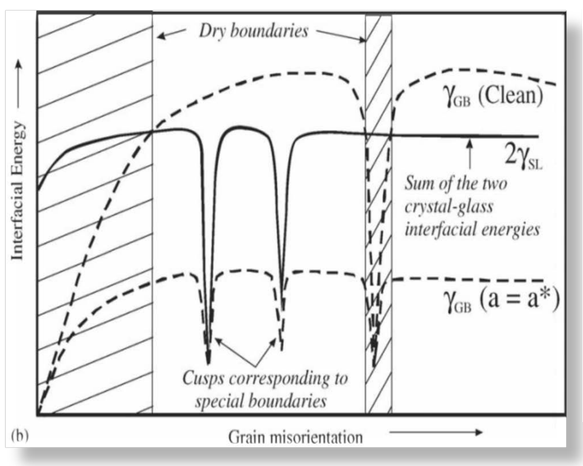
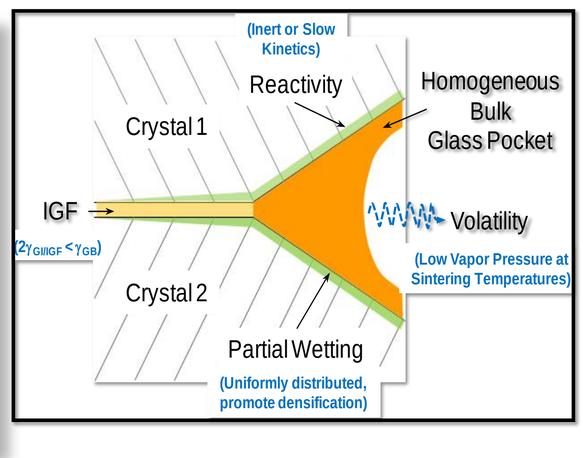
Research Objective

- **To develop atomistic and mesoscale DFT and classical molecular dynamics models to accurately capture the important physics and atomistic mechanisms that occur during ceramic processing and ultimately influence the mechanical properties and ballistic performance of B_6O**
  - **Sintering Aides**
  - **Nature of ceramic precursor and its interaction with gaseous atmospheres**
  - **Grain boundary reconstructions**
  - **Intergranular glassy films**





B_6O Challenges

- **Fracture toughness of B_6O is low (1.5 Mpa*$m^{1/2}$)**
- **Intergranular glassy films have been successfully used in other ceramic armor systems to improve the fracture toughness. However, B_6O does not naturally form an intergranular film and experimental attempts to create an IGF resulted in the glass segregating near the triple pockets.**
- **B_6O undergoes shear amorphization at high pressures and temperatures**
- **B_6O has a limited processing window (i.e. thermal decomposition) making it difficult to produce a high density ceramic with good crystallinity**
- **The role of H in catalyzing the conversion of amorphous boron to B_6O is not well understood**

Computational Challenges

- **Small system sizes (DFT < 500 atoms) and periodic boundary conditions make it difficult to create a DFT model that statistically describes the atomic reconstructions of the amorphous phases**
- **Large Combinatorial Space to explore**
- **Lack of experimental techniques at the atomistic level to validate model findings**

ARL Facilities and Capabilities Available to Support Collaborative Research

- **Processing Facilities- Large and Small Scale Powder Processing and Sintering, Hot Press, Tube Furnaces, Spark Plasma Sintering, Magnetron Sputtering onto Fluidized bed, Sol-gel**
- **Characterization Facilities- Powder XRD, X-ray Fluorescence, Scanning and Transmission Electron Microscopy, Nano-indenter, Mechanical testing facilities, FT-Raman, FTIR, Dilatometer**
- **Computational Facilities - DoD High Performance Computing (HPC) - over 2.5 billion processor hours/yr, 5 PetaFLOPS of computing capability**
- **Calculations types: Structural Optimization, Ab Initio and Classical Molecular Dynamics (MD), Metadynamics, Electronic Structure, Vibrational Modes, NMR spectra, Elastic Constants and Moduli, Formation Energies, Adsorption Energies, Cleavage Energies, Reaction and Diffusion Barriers, Transition State Searches, Phase Stability, Force Matching for MD Potential Development**
- **Codes: VASP, CASTEP, Dmol3, CP2K, Gaussian, DFT-B, Materials Studio, MeDea, LAMMPs, Pearson/ICSD/NCD Crystal Databases, Interfacial /Grain Boundary/Amorphous phase builders**

Complementary Expertise/ Facilities/ Capabilities Sought in Collaboration

- **New Approaches to Scale Up both system sizes and time-scales for first principles DFT based methods**
- **Efficient Search methods to navigate the high combinatorial chemistry space and effectively sample the potential energy surfaces in order to properly identify stable atomistic reconstructions: Genetic Algorithms, Multi-objective Optimization, Machine Learning**
- **Better Methods to capture Rare-event initiated phase transformations**
- **Novel Experimental Methods that are able to capture at the atomic scale changes in local atomic coordination between light elements and elements that have similar electronic and nuclear scattering cross-sections for computational validation**
- **Novel Experimental Methods to determine the local atomistic reconstructions along the B6O grain boundaries and the local atomic order within boron based amorphous phases**
- **In-situ Experimental methods at extreme temp/pressure**